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THREE ASPECTS OF THE STATISTICS OF DIRECTIONS.(U)

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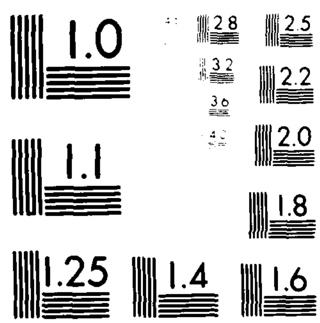

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THREE ASPECTS OF THE STATISTICS OF DIRECTIONS

by

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ABSTRACT

This paper is a selection of topics from three lectures given to the 21st Summer Research Institute of the Australian Mathematical Society. Lecture 1 gave scientific problems yielding data which are unit vectors--directions--in two and three dimensions. Methods of displaying and summarizing the data were illustrated. Lecture 2 began with the uniform distribution on a sphere of unit radius in q dimensions, then non-uniform distributions were discussed, especially those that arise in certain stochastic processes. Lecture 3 was devoted to a summary of statistical inference methods and concluded with some remarks on problems of greater generality suggested by our subject.

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1. THE STUDY OF ORIENTATION DATA.

Geology and geophysics were the first sciences to require the analysis of orientation data. In geology, the orientation of pebbles and bedding planes and other bodies gives directions with and without sense. The latter (e.g. a normal to a plane) are often called axial directions for lack of a better term. The orientation of crystals leads to rotation matrices. Here we will only consider directions i.e. (signed) unit vectors. They were first given serious study when Fisher (1953) wrote a paper for paleomagnetic workers. This was this writer's initial motivation. A survey of applications is given in Watson (1970). Later biologists interested in the homing directions of pidgeons provided two dimensional data and further problems.

As will be seen, the study of directional data forces us to modify the methods and, more interestingly, the concepts which statisticians have long used for analyzing vector data. The shift from observations $x \in \mathbb{R}^q$ to observations $x \in \Omega_q$, the surface of the unit ball in $\mathbb{R}_q$ requires new ideas. In practice, we have only so far needed methods of Ω_2 and Ω_3, the circle and sphere.

Given n data points $x_1, \ldots, x_n \in \Omega_q$, we need first methods for looking at the data. For $q=2$, the points may be marked on a circle since they are 1-1 with angles. If $[0,2\pi)$ is split into intervals, a frequency distribution is obtained. A histogram using sectors rather than boxes is called a "rose diagram"--the radius is usually proportional to the frequency but it is better to use the square root of the frequency. This transformation stabilizes the variance which makes eye-inspection for peaks or modes easier. In simple cases, the data will show only one modal

or "preferred" direction in which case we then need some measure of "dispersion" about this direction. With larger samples we might wish to use a non-parametric density estimator. We will return to these questions.

To see spherical data, it is usually only practical to look at plane projections of the points. The computer allows us easily to rotate the data--often it is mainly one hemisphere. It is then natural to use an equal area projection. If the rotated points are identified with their spherical polar angles θ(colatitude), ϕ(longitude), the spherical area element $\sin\theta d\theta d\phi$ should equal the planar area element $\rho d\rho d\phi$. Hence we find $\rho=2|\sin\theta/2|$. This Lambert projection is called the Schmidt net in Geology.

If the data $x_1,\ldots,x_n$ seems to be uni-modal, it is natural to define the modal-direction to be the unit vector $\hat{\mu}$ parallel to $R=\sum_1^n x_j$, the vector resultant or sum of the data. If the data is widely dispersed, the length $\|R\|$ of R will be much smaller than n . If it is tightly clustered about $\hat{\mu}$, $\|R\|$ will be almost n . Hence $n-\|R\|$ is a measure of dispersion of the data set, an analogue in fact of the reciprocal $\Sigma(x_j-\bar{x})^2$ for the familiar case when the x_j are real numbers. So we may expect that $\hat{\mu}$ and $\frac{n-1}{n-\|R\|}$ will in some way play the roles of the familiar mean and variance. Of course if the data cluster is not fairly rotationally symmetric about $\hat{\mu}$, more than one number will be needed to describe its dispersion.

If the data points x_j are regarded as unit masses, $\frac{1}{n}\sum_1^n x_j$ is their center of gravity. As we have just seen, the position of this point within the sphere tells us something about the distribution of the data. The moment of inertia clearly tells us something more. This leads us to suggest

the computation of

$$M = \sum_1^n x_j x_j'$$

where x_j' is the transpose of the column vector x_j . For the value of $\nu'M\nu=\Sigma(\nu'x_j)^2$ will change as the unit vector ν varies. The stationary values are the eigen values of M . If, for example, the data points lie fairly uniformly around a great circle, one eigen value will be much smaller than the others which will be nearly equal--for there is a ν nearly orthogonal to all the data and this is the eigen vector associated with the minimum eigenvalue. The reader can easily see what would be suggested by equal eigen values or one dominating eigen value. Note that trace $M=\sum_1^n$ trace $x_j x_j' = \sum_1^n x_j' x_j = n$.

Thus one should add to the rotation and projection program, these trivial computations and have the results printed out below the pictures which we obtain by making hard copies from a Textronics (C.R.T.) terminal.

With real data, power moments are sometimes used. For circular data $x_j \langle\!-\!\rangle \theta_j$, it is even more natural to use $\frac{1}{n}\sum_1^n \exp ik\theta_j = (\frac{1}{n}\Sigma\cos k\theta_j \; , \frac{1}{n}\Sigma\sin k\theta_j)$ for integer k because for any density on the circle with a Fourier series representation $f(\theta)=\sum_{-\infty}^{\infty} c_m \exp im\theta$, the expectation of $n^{-1}\sum_1^n \exp ik\theta_j$ is c_{-k} . This leads to a non-parametric density estimator--see Watson (1969). For the sphere, spherical harmonics may be used in a similar way.

For data $x_1,\ldots,x_n$ on Ω_q , a non-parametric density estimator of the kernel type may be constructed as follows. Let $\delta_n(x;z)$ be a sequence of probability densities on Ω_q corresponding to probability distributions which concentrate on the fixed unit vector z as $n\to\infty$. For example the

density

$$e(\alpha_n)\exp\alpha_n x'z \tag{1}$$

could be used with $\alpha_n\to\infty$ as $n\to\infty$. Then the estimator

$$\hat{f}_n(z) = \frac{1}{n}\sum_{j=1}^{n}\delta_n(x_j;z) \tag{2}$$

will become unbiased as $n\to\infty$ since

$$E\hat{f}_n(z) = \int\delta_n(x;z)f(x)d\omega$$

where $d\omega$ is the area element on Ωq . Then

$$E\hat{f}_n(z)\to f(z) \quad , \quad \text{as} \quad n\to\infty \quad .$$

Furthermore

$$\begin{aligned} \operatorname{var}\hat{f}_n(z) &= \frac{1}{n}\operatorname{var}\delta_n(X;z) \\ &= \frac{1}{n}\{\int\delta_n^2(x;z)f(z)d\omega - (E\hat{f}_n(z))^2\} \ , \\ &\sim \frac{f(z)}{n}\int\delta_n^2(x;z)d\omega \ , \qquad \text{as} \quad n\to\infty \end{aligned}$$

so that $E(\hat{f}_n(z)-f(z))^2\to 0$ provided that $\int\delta_n^2(x;z)d\omega$ tends to infinity slower than n .

With the choice (1), the estimator (2) is easily programmed. To see the result we also need a contouring program. The contours may be shown, along with the original data points, by using the Lambert projection mentioned above. The neatest method uses overlaid transparencies. The notion of a kernel estimator seems to occur first in Watson (1970) but the first implementation, much as I have described here, seems to be in a thesis on polar wandering by Alstine (1979).

In Lecture 1, all these methods were illustrated on a data set--the normals to the orbits of all the comets in the latest Smithsonian Catalogue (1979).

As will be explained in the next section, for uni-modal distributions with rotational symmetry, the most commonest model is the density

$$c(\kappa) \exp \kappa\, x'\mu \qquad (3)$$

where μ is the modal direction and κ is an accuracy parameter. It is therefore important to have a quick method to check the fit of (3) to data. For $q=3$, it will be shown below that:

$$\phi \text{ is uniformly distributed on } [0,2\pi) \qquad (4)$$

independently of

$$\exp-\kappa(1-\cos\theta) \text{ which is approximately uniformly distributed on } [0,1]. \qquad (5)$$

It is easy to check uniformity--we may use histograms, (or their computer form, stem & leaf plots), P-P or Q-Q plots (essentially the same for uniform distributions). To carry this out for (5), it is necessary to use an estimator of κ e.g. the estimator $(n-1)(n-|R|)^{-1}$ may be used. For $q=2$, (3) may be written

$$\frac{1}{2\pi I_0(\kappa)} \exp\kappa\cos\theta \qquad (6)$$

where $\cos\theta = x'\mu$ and $I_0(\kappa)$ is a Bessel function. Using the maximum likelihood estimators of μ and κ (see Section 3), it is easy to compute an approximate P-P plot.

In Lecture 1, these quick checks of (3) for $q=2,3$ were illustrated on the comet data and no subset of comets was found to fit this distribution.

2. PROBABILITY DISTRIBUTIONS ON Ωq

In the notation of Müller (1966), let $d\omega_q$ be the area element on $\Omega_q = \{x | x\epsilon \mathbb{R}^q, ||x|| = 1\}$, $|\Omega_q|$ be the area of Ω_q . If $\varepsilon_1,\ldots,\varepsilon_q$ are orthonormal vectors in $\mathbb{R}^q$, and $x\epsilon\Omega_q$, then

$$x = t\ \varepsilon_q + \sqrt{1-t^2}\ \xi_{q-1}$$

where $t=x'\varepsilon_q$, ξ_{q-1} = unit vector in the space spanned by $\varepsilon_1,\ldots,\varepsilon_q$ and

$$d\omega_q = (1-t^2)^{(q-3)/2} dt\ d\omega_{q-1} \quad .$$

(The special case $d\omega_3 = d\cos\theta d\phi$ is well known.) Thus

$$\omega_q = \omega_{q-1} \int_{-1}^{1} (1-t^2)^{(q-3)/2} dt \ ,$$

so that

$$\omega_q = 2\pi^{q/2} / \Gamma(q/2) \quad .$$

The characteristic function, or Fourier transform, of any density $f(x)$ on Ω_q is given by

$$E(\exp i\theta' x) = \int_{\Omega_q} \exp i\theta' x\ f(x) d\omega_q \ , \ \theta\epsilon\mathbb{R}^q \quad .$$

The fundamental distribution on Ω_q is the <u>uniform distribution</u> with density $|\Omega_q|^{-1}$. Setting $\Theta=\theta a$, $a\epsilon\Omega_q$, $a'x=t$, we find that

$$E(\exp i\theta t) = \frac{\omega_{q-1}}{\omega_q} \frac{\pi^{1/2} J_\nu(\theta)\ \Gamma(\nu+1/2)}{(\theta/2)^\nu} \qquad (7)$$

where $\nu=(q-1)/2$ and $J_\nu(\theta)$ is a Bessel function.

If now $Y=a'(\sum_1^n x_j)=t_1+\ldots+t_n$, the characteristic function of Y is the n-th power of (7). Hence the density of Y may be formally obtained by inverting the n-th power of (7). The distribution of $\|\sum_1^n x_j\|$ can then be deduced from the additional observation that the direction of $\sum_1^n x_j$ is uniform.

While the exact distribution of the length of the sum of n independent and uniformly distributed vectors may be deduced this way, it is an analytically awkward result. However it is easy to obtain an excellent approximation when n is not small. For

$$\|\Sigma x_j\|^2 = Z_1^2 +\ldots+ Z_q^2 = \|Z\|^2$$

where Z_k = sum of the k-th coordinates of $x_1,\ldots,x_n$. By the Central Limit Theorem, these sums become Gaussian. For all n , the mean vector and covariance matrix of Z are respectively 0, nI_q/q . Hence the asymptotic distribution of qR^2/n is the chi-square distribution with q degrees of freedom. This result for $q=2,3$ goes back to Rayleigh (1880,1919) and is central to the problem of random flights, or as it was first called by Pearson (1905), random walks. The flights were of mosquitoes and the problem was raised in this form by Sir Ronald Ross' speculations of the spread of fevers. Rayleigh was concerned with the random phases of sound.

The random walks not only serve as a basic model in many areas of science but have deep and wide connections with mathematics. The literature on them is vast.

Non-uniform distributions are interesting to statisticians for one of several reasons:

(i) they fit data

(ii) they arise from stochastic modelling and

(iii) it is easy to derive inference methods for them.

With the advent of computers (iii) is less compelling than it once was. Further with the mathematical techniques available now for large sample theory, (iii) is also less important.

Densities which have been suggested with an eye on (i) and (iii) are: $x, a \in \Omega_q$

$$f \propto \exp \kappa a'x \quad , \tag{8}$$

(rotational symmetry about a single mode)

$$f \propto \exp \kappa (a'x)^2 \tag{9}$$

(two equal but opposite modes $\kappa > o$, a girdle distribution $\kappa < o$, rotational symmetry)

$$f \propto \exp \kappa a'x + \lambda (a'x)^2 \tag{10}$$

(two unequal but opposite clusters, rotational symmetry)

The use of the exponential rather than a more general function is due to (iii) for the joint density of independent observations is the product of the densities--this will become clearer to non-statisticians in Section 3.

The modelling approach--asking what processes actually led to the data--often reveals that the directions are in fact the directions of random vectors whose lengths have been ignored. This is so in paleomagnetism for

example. Let X be a random vector in $\mathbb{R}^q$ with density $f(x)$ with length r so $X=\gamma\ell$ where $\|\ell\|=1$ so $\ell \in \Omega_q$. Then the density of ℓ is

$$g(\ell) = \int_0^\infty f(r\ell)r^{q-1}dr \tag{11}$$

For example if X is Gaussian with mean vector μ and covariance matrix Σ, the density g is then called the angular Gaussian. Special cases have special names.

Work in structural geology led the writer to consider $Y=TX$ where $|T|\equiv\det T>0$. Setting $Y=\ddot{r}m$ with $m\in\Omega_q$, it follows from (8) that the density of m, $h(m)$ is defined by

$$h(m) = \frac{1}{|T|}\,\frac{g(T^{-1}m/\|T^{-1}m\|)}{\|T^{-1}m\|^q} \tag{12}$$

The righthand side of (12) is unchanged if $T\to kT$ so there is no loss of generality in taking $|T|=1$. The transformation $Y=TX$ is a homogeneous strain so we see that if only the orientations are known, one may not determine the dilatation $|T|$ of the strain.

A most elegant formula is easily deduced from (12),

$$\int_{\Omega_q} \|T^{-1}m\|^{-q}d\omega_q = \omega_q|\det T| \tag{13}$$

There are many more interesting formulae of this type. Again, we may derive the density

$$g(\ell) = \frac{|T|}{\omega_q}\,\frac{1}{\|T\ell\|^q} \quad , \quad |T|>0 \ , \ \ell \in \Omega q$$

$$= g(-\ell) \quad . \tag{14}$$

If we may set $T=\Sigma^{-1/2}$, Σ positive definite, (14) becomes

$$g(\ell) = \frac{\omega_q^{-1}}{|\Sigma|^{1/2}} \frac{1}{(\ell'\Sigma^{-1}\ell)^q} \tag{15}$$

which has been noted before by several authors (e.g. King (1980).

The above paragraph has used the marginal density of vectors, integrating out their length. Conditional distributions (given that their length is unity) don't seem to arise in modelling but are of mathematical interest. For example if X is Gaussian mean μ covariance $\sigma^2 I_q$, the density function of X is proportional to

$$\exp - \frac{1}{2\sigma^2} (x'x - 2x'\mu + \mu'\mu)$$

so the conditional distribution of x , given $||x||=1$ is proportional to

$$\exp \frac{1}{\sigma^2} x'\mu , \tag{16}$$

as was first pointed out by Fisher.

This density (16) has arisen above--(8). For $q=2$ it was first suggested by vonMises (1918). For $q=2,3$, it was suggested and briefly studied by Arnold (1941). For $q=3$, it was the basis of Fisher's (1953) paper.

Another distribution whose mathematical form is convenient for statistical inference has

$$f \propto \exp x'Kx \qquad (K \text{ a symmetric matrix})$$

and was studied by Bingham (1974). Density (9) was suggested by Watson

(1965) and Scheidegger (1965), density (10) appears in Fraser (1979).

A fertile source of distributions is Brownian motion. If a particle moves in $\mathbb{R}^1$ with independent steps $dx=\xi dt$, $E\xi=0$, $E\xi^2=\sigma^2$ at time steps dt , the probability density $\phi(x,t)$ of its position x at time t is given by

$$\phi(x,t) = \frac{1}{\sqrt{2\pi}\,\sqrt{\sigma^2 t}}\ \exp - \frac{x^2}{2\sigma^2 t} \tag{17}$$

by well known arguments. If the same motion occurs on the circumference of a circle of unit radius, the position θ of the particle at time t is given by

$$f(\theta,t) = \sum_{-\infty}^{\infty} \phi(\theta+2\pi k,t)\ , \tag{18}$$

$$= \frac{1}{2\pi}\,\Sigma\, \exp(-m^2\sigma^2 t)\exp im\theta \quad ,$$

$$= \frac{1}{2\pi}\,(1+2\sum_{1}^{\infty}\exp(-m^2\sigma^2 t)\cos m\theta)\quad . \tag{19}$$

Because of (18), $f(\theta,t)$ is often called the "rolled-up" or "wrapped" normal density. (19) may be contrasted with the von Mises density which has the Fourier series

$$\frac{1}{2\pi}\,(1+2\sum_{1}^{\infty}\frac{I_m(\kappa)}{I_0(\kappa)}\cos m\theta) \tag{20}$$

Both (19) and (20) have modes at $\theta=0$ and the agreement is remarkable if the coefficients of $\cos\theta$ are identified i.e.

$$e^{-\sigma^2 t} = I_1(\kappa)/I_0(\kappa) \tag{21}$$

It may be shown (Hartman and Watson (1976)) that stopping the circular diffusion at a random time, the density (20) may be obtained exactly. Pitman and Yor (1980) have shown that there is more than one such stopping time distribution. Similar results are true for Ω_q .

It is also possible to obtain the densities (8) and (9) by other diffusion models. For example if we consider, following Kent (1976), a circular diffusion like the previous one but with a drift term so that the step in dt is

$$d\theta = -\kappa\sin\theta\, dt + \xi\sqrt{dt}$$

then, as $t\to\infty$, the chance that the particle will be found in the interval $(\theta,\theta+d\theta)$ tends to $d\theta\exp\kappa\cos\theta$, the von Mises density. If the step is given by

$$d\theta = -\kappa\sin^2\theta\, dt + \xi\sqrt{dt} ,$$

the limiting density is proportional to $\exp\kappa\cos^2\theta$, which is the $q=2$ form of (9). An intuitive proof of the first of these results follows from considering a physical diffusion in a circular pipe of cross-section area A. Let the concentration of particles at θ be $f(\theta)$, then by Fick's law the diffusion forward across A at θ is $-AD\partial f/\partial\theta$, where D is a diffusion coefficient. If the medium has a velocity $v(\theta)$ at θ , the transport across A is $Af(\theta)v(\theta)$. At equilibrium the number of particles in the pipe between θ and $\theta+d\theta$ must be constant. Hence

$$\left(-AD\frac{\partial f}{\partial\theta}\Big|_{\theta} + AD\frac{\partial f}{\partial\theta}\Big|_{\theta+d\theta}\right)+\left(Afv|_{\theta}-Afv|_{\theta+d\theta}\right) = 0$$

or

$$Df''(\nu f)' = 0 \tag{22}$$

Setting $\nu(\theta)=-\kappa\sin\theta$ and $D=1$, the solution f is seen to be proportional to $\exp\kappa\cos\theta$.

This argument is intimately connected with a well-known result in statistical mechanics (see e.g. Joos (1947)) on the distribution of thermally agitated magnetic dipoles, moment m, in a parallel field H. There it is found that $\kappa=mH/kT$ where T is the absolute temperature and k here stands for Boltzmann's constant.

In the discussion of Kendall (1974), Reuter suggested another diffusion model for (8). Let particles be steadily released from the origin of the sphere $\|x\|=1$ and record where they first hit Ω_q. The distribution of first hits will be uniform without any drift but if the drift is constant it will have the density (8). To get an intuitive proof of this result, let f be the equilibrium concentration of particles at any point in or on the sphere when they are steadily produced at the rate of 1 per unit time at the origin. Let them diffuse (but not interact with each other) in a medium that moves with an arbitrary velocity $v(x)$. The answer we seek is $\partial f/\partial n|_{\Omega_q}$, the normal derivative of f on $\|x\|=1$. If V is any small volume within the sphere with boundary ∂V, the loss of particles from V due to transport is

$$\int_{\partial V} n\cdot(vf)dS \sim |V|\operatorname{div}(vf)$$

where n is an outward normal and dS an area element on ∂V. The gain due to diffusion is

$$\int_{\partial V} \frac{\partial f}{\partial n}\, dS \sim |V|\nabla^2 f$$

If V is a vanishingly small volume that does not include the origin and equilibrium is attained, the concentration f satisfies

$$\begin{aligned} {}^2 f - \operatorname{div} v\, f = 0 \,, &\qquad \|x\| \neq 0,1 \\ f = 0 \,, &\qquad \|x\| = 1 \end{aligned} \tag{23}$$

This is, of course, a generalization of (22). To ensure a suitable source of particles at the origin we must demand that

$$\begin{aligned} f &\to \frac{1}{\omega_q(q-2)} \frac{1}{r^{q-2}} \qquad (q \neq 2) \;, \\ &\to \frac{1}{2\pi} \log \frac{1}{r} \qquad (q=2) \;, \end{aligned}$$

as $r = \|x\| \to 0$.

For the special case, $q=2$, $v_x = c$, $v_y = 0$, we may try $f = \exp(kx)\, g(x,y)$ in (23). It is readily seen that if we choose $k = c/2$, g must satisfy

$$\left.\begin{aligned} &{}^2 g = \frac{c^2}{4} g \;, \\ &g = 0 \;,\; r^2 = x^2 + y^2 = 1 \;, \\ &g \sim \frac{1}{2\pi} \log \frac{1}{r} \;,\; r \to 0 \end{aligned}\right\} \tag{24}$$

But (24) implies that g is a function only of r . Hence

$$f(x,y) = g(r) \exp \frac{c}{2} r\cos\theta \;,$$

so that $\partial f/\partial r$ on the boundary $r=1$ is proportional to $\exp(c/2 \cos\theta)$. Inspection shows that the proof trivially extends to any number of q dimensions. Finally by choosing other velocity fields, other distributions on

the sphere may be obtained. This is technically difficult unless the velocity fields are generated by a potential as in classical hydrodynamics.

Lecture 2 concluded with visual comparisons of many distributions on the circle and sphere.

3. INFERENCE PROBLEMS ON Ω_q

3.1 Introduction

Testing whether a random sample of directions $x_1,\ldots,x_n$ has been drawn from the uniform distribution is possibly the oldest significance test problem. Bernoulli (1734) considered whether the orientations of the planetary orbits were random. Watson (1970) reconsidered the problem with modern data and used the normals to the orbital planes, directed by the righthand rule. An intuitive and approximate test, using the length of the vector sum 7.13 of the 9 normals, may be based on Rayleigh's result. Naturally the null hypothesis is strongly rejected. By using Neyman-Pearson theory, elegant and sensitive methods may be tailor-made when one has certain alternatives in mind. These will be discussed in Section 3.4.

Much of the literature is concerned with estimation and testing problems when the data are assumed to be drawn from the von Mises-Arnold-Fisher density (8). This will be briefly outlined in Section 3.2. Similar theory and methods have been developed for other specific densities but space does not permit mentioning them.

One is rarely certain that a specific distributional form obtains so all methods of analysis should not be too sensitive i.e., they should be robust. One may check the behavior, by computer simulation, of the methods mentioned in the previous paragraph to see how resistant they are to changes in distributional form and outliers in the data. Or better, try to design new methods of analysis that will be robust. Another method is to make few distributional assumptions but to assume that the samples are large enough to permit fairly good approximations to be made--essentially that

a Central Limit Theorem effect will operate. This is the topic of Section 3.3

3.2 Inference for the von-Mises-Arnold-Fisher distribution

The flavor of this topic is best seen by discussing only the case $q=3$. Then the density on the sphere Ω_3 is

$$f(x) = \frac{\kappa}{4\pi \sinh\kappa} \exp \kappa\, x'a \quad , \quad \kappa \geq 0 \tag{25}$$

Clearly when $\kappa=0$, this becomes the uniform density, $(4\pi)^{-1}$. As $\kappa \to \infty$, all the probability concentrates about the mode a. The distribution is always rotationally symmetrical about a. Of course $||a||=1$.

If a sample $x_1, \ldots, x_n$ is drawn from (25), the logarithm of the likelihood of the data is, to a constant,

$$n \log(\kappa/\sinh\kappa) + \kappa\, (\Sigma x_i)'a \tag{26}$$

This is maximized by choosing a parallel to $\underline{R}=\Sigma x_i$. Hence the maximum likelihood estimator $\hat{a}$ of a is the direction of $\underline{R}=\Sigma x_i$, the intuitive estimator we met in Section 1. Thus $\hat{a}=\underline{R}/R$, where $R=||\Sigma x_i||$. The value of κ which then maximizes (26) with $\hat{a}$ instead of a, $\hat{\kappa}$ say, satisfies

$$\coth \hat{\kappa} - \frac{1}{\hat{\kappa}} = \frac{R}{n} \quad . \tag{27}$$

If $\hat{\kappa}>3$ and n is not too small, $\hat{\kappa} \approx k$ where

$$k = \frac{n-1}{n-R} \tag{28}$$

the intuitive accuracy estimator we met in Section 1. If a were known, and we write $X = a'\underline{R}$, the estimator of κ would be fairly accurately

$$k' = \frac{n}{n-\chi} \tag{29}$$

It is of course trivial to compute the exact maximum likelihood (m.ℓ.) estimators.

To find a confidence cone for the true modal direction a , we consider the problem of testing the null hypothesis H_0 that the true modal direction is a . This is how the analogous problem for the linear normal distribution is solved. There one can consider the analysis of variance identity

$$\Sigma(x_j-\mu_0)^2 = \Sigma(x_j-\bar{x})^2 + n(\bar{x}-\mu_0)^2 \tag{30}$$

along with the distributional identity

$$\sigma^2\chi^2_n = \sigma^2\chi^2_{n-1} + \sigma^2\chi^2_1 \tag{31}$$

where the terms on the righthand side of (31) are independent. To check where $\bar{x}$ is too far from μ_0 for the null hypothesis to be likely, we notice that the ratio

$$\frac{n(\bar{x}-\mu_0)^2}{\Sigma(x_j-\bar{x})^2} = \frac{\chi^2_1}{\chi^2_{n-1}} \tag{32}$$

whose distribution is free of unknown parameters. In fact, if one multiplies both sides of (32) by (n-1), the lefthand side is t^2 and the righthand side is distributed as $F_{1,n-1}$.

Returning to our problem, the analogue of (30) is

$$n - \chi = n-R + R-\chi \tag{33}$$

because we saw in Section 1 that n-X and n-R were measures of dispersion of the data about the true and estimated modes. In the next paragraph we

will see that we may assert, if κ is not small, that approximately

$$2\kappa(n-X) \approx \chi^2_{2n}\ ,\ 2\kappa(n-R) \approx \chi^2_{2(n-1)}\ ,\ 2\kappa(R-X) \approx \chi^2_2 \tag{34}$$

and that the last two expressions are independent. Hence we have the analogue of (32)

$$\frac{R-X}{N-R} \simeq \frac{\chi^2_2}{\chi^2_{2(n-1)}} \tag{35}$$

which, if multiplied by $(n-1)$ leads to the $F_{2,2(n-1)}$ distribution. Large values of (32) and (35) both lead us to reject the null hypothesis. Since $X=R\cos\theta$ where θ is the angle between the true and sample modal directions, the lefthand side of (33) is

$$R(1-\cos\theta)/(N-R)$$

so that the semi-angle θ_{95} of a 95% confidence cone is defined, to good accuracy, by the equation

$$(n-1)\frac{(1-\cos\theta)\ R}{N-R} = F_{2,2(n-1)}\quad(95\%) \tag{36}$$

To justify (34), we note that the Fisher density (25), put in spherical polar angles with $x'a=\cos\theta$, yields a joint density of θ,ϕ

$$\frac{\kappa}{4\pi\sinh\kappa}\exp(\kappa\cos\theta)\sin\theta\ ,$$

$$\approx \kappa\, e^{-\kappa(1-\cos\theta)}\sin\theta\cdot\frac{1}{2\pi}\ ,$$

if κ is large. Thus ϕ is uniformly distributed on $[0,2\pi)$ independently of θ and $w=\kappa(1-\cos\theta)$ has a standard exponential distribution. Thus

$2w = \chi_2^2$ and $\exp(-\omega)$ has a uniform distribution on $[0,1]$. These results were needed in Section 1 to justify a rough goodness of fit procedure. The assertions (34) now become good guesses. In fact one must verify all this intuitive approach by mundane methods. But if one understands it one can guess how much more complicated problems should and can be solved e.g. in the lectures this was illustrated with two sample problems. This adds insights instead of merely mechanically applying classical inference methods to derive procedures.

Other fully specified distributions may be more appropriate than (25) in which case similar techniques may be used.

Mardia (1972) is primarily a summary of this aspect of our subject, for $q=2,3$.

3.3 Robust methods

One is rarely confident that one's data is a sample from a specific distribution so it is ridiculous to use an analysis which is sensitive to small changes in the parental distributional form. Any procedure (e.g. that in (36)) can be checked by computer simulation. One simply invents a distribution, draws random samples from it, computesthe statistic again and again and compares the observed with theoretical proportions. I found e.g. that the test procedure implied by (36) was very robust but that related tests for comparing κ's were not--see Watson (1967).

Instead of checking whether a procedure is robust, it perhaps better to set out to design procedures which <u>will</u> be robust. This is an active research area nowadays in which Huber, Hampel and Tukey have provided key ideas.

The most studied problem is: how to make sound inferences about the center of a symmetric density on the line. It is assumed that the density behaves, around the center, like the Gaussian but may further out have much heavier tails.

The analogous problem on Ω_3 would be to assume a rotationally symmetric distribution

$$f = c(\kappa;f_0)f_0(\kappa\, a'x) \tag{37}$$

If f_0 is exp this (25). If the m.ℓ. method is applied to (37) we find that the estimator of a, $\hat{a}$, must be parallel to

$$\sum_{j=1}^{n} \frac{f_0'(\kappa\, \hat{a}'x_j)}{f_0(\kappa\, \hat{a}'x_j)}\, x_j \quad , \tag{38}$$

in contrast to Σx_j for the Fisher distribution. The trick now is to design this "weighted" sum so that it is not too sensitive to very aberrant vectors. This is one of my current research projects.

If large samples are available, it is intuitively clear that we should be able to learn from the data itself something about the shape of the distribution sampled and so to design methods that will be effective whatever the true distribution is. No such "adaptive" methods now exist.

For large n, $n^{-1/2}\sum_{1}^{n} x_j$ will have approximately a q dimensional Gaussian distribution with a mean μ and covariance Σ defined by

$$\mu = \int_{\Omega_q} x\, f\, d\omega_q \;,\; \Sigma = \int_{\Omega_q} (x-\mu)(x-\mu)'f d\omega_q \tag{39}$$

The approach was first use[illegible] Sengupta and J.S. Rao (1966) and in the latter thesis (Rao, 1969), compared with my analysis of variance (explained briefly

in the last section) when f is the von-Mises distribution. However no assumptions about f need to be made and no effort was made to estimate f or to "tailor" the analysis to be particularly effective when f is "near" the $\exp\kappa x'a$ form.

Wellner (1980), in an unpublished paper, took a similar approach but assumed that the data came from an axially symmetric distribution on Ω_3 i.e. that

$$f = f(a'x) \quad . \tag{40}$$

For general q, it is easy to prove that, instead of (39),

$$\left.\begin{aligned} \mu &= \rho a \quad , \ |\rho| \leq 1 \\ \Sigma &= \alpha^2 aa' + \beta^2 (I_q - aa') \quad , \end{aligned}\right\} \tag{41}$$

where α and β are simple functions of $E(a'x)$, $E(a'x)^2$. The procedures which result will be more efficient than those of Rao if the rotational symmetry is true.

In fact the commonest deviation from the von-Mises, Arnold, Fisher distribution is lack of rotational symmetry but, except for my simulation studies, there is no published work on this problem. Oval shaped clusters of data on the sphere in paleomagnetism are often attributed to a mixture of distributions with different modal vectors. Again, no studies have been made of the effect of lack of independence on estimators of modal directions--this can have a disastrous effect in linear problems and may be expected to do the same on the sphere.

3.4 Testing whether f is uniform

If on the null hypothesis H_0, $f=\omega_q^{-1}$ and on the alternative H_1, $f=f_1$, then the Neyman-Pearson Lemma tells us to reject H_0 in favor of H_1 if $\prod_{j=1}^{n} f_1(x_j)$ is too large. Suppose $f_1 = f(0_q x)$ where 0_q is a rotation matrix. If 0_q is unknown, it is reasonable to demand a test statistic which does not depend upon what 0_q is i.e. to demand an invariant test. This leads to the test statistic

$$\int \prod_{j=1}^{n} f(0_q x_j) d0_q = \operatorname*{ave}_{0_q} \Pi f(0_q x_j) \tag{42}$$

The statistic (42) may be trivially evaluated when $q=2$ because it will naturally be written

$$\int_0^{2\pi} \prod_1^n f(\theta_j+\phi)d\phi \tag{43}$$

In the particular case where $f(\theta+\phi) = \exp\kappa\cos(\theta+\phi)/2\pi\ I_0(\kappa)$, (43) is proportional to $I_0(\kappa R)$ which (since $\kappa>0$) increases monotonically with R (the length of the sum of the data vectors). Thus we can assert that in this case the so-called Rayleigh test--reject uniformity if R is too large--is the best invariant test. This test makes intuitive sense whenever the alternative is uni-modal.

If the alternative density is very far from uniformity it should be easy to design a sensitive test when one has enough data. But if the alternative density is close to uniformity, more care is obviously required. Beran (1968) gave an elegant theory for testing for uniformity on compact homogeneous spaces. To sketch this in our setting, we suppose a sequence of alternatives to uniformity defined by

$$f_\kappa(x) = \omega_q^{-1} + \kappa\{f(0_q x) - \omega_q^{-1}\} \quad , \qquad \kappa\to 0 \quad . \tag{44}$$

The integral of $f_\kappa(x)$ over Ω_q will be unity and $f_\kappa(x)$ will be non-negative for κ small enough if $f(x)$ is bounded on Ω_q . Of course, $f_\kappa(x) \to \omega_q^{-1}$, the uniform density as $\kappa\to 0$.

Setting $\lambda=\kappa\omega_q$, Ave $\Pi f(0_q x_j)$ is proportional to

$$\text{Ave } \Pi \ (1 + \lambda\{\omega_q \ f(0_q x_j) - 1\} \ )$$

$$= \text{Ave } [1 + \lambda \sum_j \{\omega_q \ f \ (0_q x_j)-1\} + \lambda^2 \sum\sum_{j\neq k} (\omega_q f(0_q x_j)-1)(\omega_q f(0_q x_k-1)]$$

plus smaller terms. *The average of the coefficient of* λ *is zero and the* coefficient of λ^2 may be simplified by the identity $\Sigma\Sigma a_j a_k = (\Sigma a_j)^2 - a_j^2$. Noting that

$$\text{Ave } (\omega_q f(0_q x_j) - \ )^2 \ \text{ independent of } \ x_j \quad ,$$

Beran thus shows that the best invariant test for this sequence of local alternative hypotheses is based on large values of

$$\underset{0_q}{\text{Ave}} \ [\sum_j \{\omega_q f(0_q x_j)-1\} \ ]^2 \tag{45}$$

To complete the test we need the distribution of (45) when the data actually come from a uniform distribution. This is naturally calculated by Fourier methods. If we take a circle of unit perimeter and set $f(\theta) = c_m \exp i2\pi m\theta$, it is easily shown that

$$\Sigma\{f(\theta_j+\phi)-1\} = \sum_{m\neq 0} c_m \exp i2\pi\phi m \sum_j \exp i2\pi m\theta_j \quad , \tag{46}$$

$$\int_0^1 [\Sigma\{f(\theta_j+\phi)-1\}]^2 d\phi = 2 \sum_1^\infty |c_m|^2 |\sum_j \exp i2\pi m\theta_j|^2 \quad . \tag{47}$$

Now it may be shown that, as $n\to\infty$,

$$\frac{2}{n} |\sum_j \exp i2\pi m\theta_j|^2 \to \chi_2^2 \qquad , m=1,2,\ldots, \tag{48}$$

and that these random variables are independent. Hence the asymptotic distribution of

$$\frac{1}{n} \int_0^1 [\Sigma\{f(\theta_j+\phi)-1\}]^2 d\phi \tag{49}$$

is that of

$$\sum_1^\infty |c_m|^2 \chi_2^2 \quad . \tag{50}$$

The statistic (47) has an intuitive interpretation. We will not pause to give this or to explain how the distribution of (50) may be obtained. The U_n^2 statistic of Watson (1961) is a special case of (50) and is a circular variant of the Cramér-von Mises statistic.

Beran's work was motivated by Ajne (1968) who defined special sequences of local and distant alternatives, and Watson's use of Fourier methods. It will be noted that to get statistics of the Kolmogorov type, which use the supremum, it is necessary to use distant alternatives. This was explored

further in Watson (1974), in the E.J.G. Pitman Festschrift.

An important point to notice here is that sample distribution functions will not usually arise--they are natural only on the line. Further, if the circle is a guide, supremum type tests can only be justified on rather absurd grounds. However their mathematical interest has led to an enormous literature.

The topic of testing uniformity is one of great mathematical interest since it may be treated in greater generality than many statistical problems. The papers of Giné (1975), Wellner (1979), Prentice (1978) give a flavor of this work.

4. CONCLUDING REMARKS

In these three lectures, I have tried to illustrate, by reference to directional data, the three sides of statistics:

- Data Analysis - especially the use of computers and graphics,
- Modelling - use of stochastic processes,
- Inference - Estimation and Testing, Robustness.

I have made no effort to cover the entire spectrum of problems, solved and unsolved, that arise with directional data. Many topics which I consider to be important and interesting have been ignored.

Further we have seen that linear and spherical data must be treated differently--the mathematical structure of the sample and parameter spaces plays an essential role. For data in $\mathbb{R}^q$, we have well defined notions of mean, variance, covariance, correlation. These quantities are still not satisfactorily defined on Ω_q. Again for parameters in $\mathbb{R}^q$ we have (modulo some technical arguments) firm ideas about what we mean by a "good" or "best" estimator. On Ω_q, we have NONE!

We have seen how Pitman's early work on location and scale parameters, and invariance can be greatly extended to data in homogeneous spaces. A greatly extended general theory of statistics could be developed. The very simple practical problems with unit vectors with which we began have led us into unknown territory.

Finally I would like to thank Prof. D.R. McNeil for bringing me back to my native land and the Australian Mathematical Society for the invitation to speak to their 21st Summer Research Institute.

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This paper is a selection of topics from three lectures given to the 21st Summer Research Institute of the Australian Mathematical Society. Lecture 1 gave scientific problems yielding data which are unit vectors--directions--in two and three dimensions. Methods of displaying and summarizing the data were illustrated. Lecture 2 began with the uniform distribution on a sphere of unit radius in q dimensions, then non-uniform distributions were discussed, especially those that arise in certain stochastic processes. (OVER) next page

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Lecture 3 was devoted to a summary of statistical inference methods and concluded with some remarks on problems of greater generality suggested by our subject.

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